Model Summary:

Model information:
- Modelled residue range: 3 to 363
- Based on template: 2efjA (2.00 Å)

Remark: No search for template was performed. Only user specified template was used for modelling.

Sequence Identity [%]: 34.324
Evalue: 0

Quaternary structure information:
- Template (2efj): DIMER
- Model built: SINGLE CHAIN

Ligand information:
- Ligands in the template: 37T: 1, ALA: 1.
- Ligands in the model: none.

Quality information:
- QMEAN Z-Score: -3.396

Global Model Quality Estimation:

QMEAN4 global scores:
- QMEANscore4: 0.565
- Z-Score: -3.396

QMEAN4 global scores:
The QMEAN4 score is a composite score consisting of a linear combination of 4 statistical potential terms (estimated model reliability between 0-1). The pseudo-energies of the contributing terms are given below together with their Z-scores with respect to scores obtained for high-resolution experimental structures of similar size solved by X-ray crystallography:

<table>
<thead>
<tr>
<th>Scoring function term</th>
<th>Raw score</th>
<th>Z-score</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_beta interaction energy</td>
<td>-113.31</td>
<td>-0.77</td>
</tr>
<tr>
<td>All-atom pairwise energy</td>
<td>-8826.12</td>
<td>-0.72</td>
</tr>
<tr>
<td>Solvation energy</td>
<td>-26.53</td>
<td>-0.90</td>
</tr>
<tr>
<td>Torsion angle energy</td>
<td>-31.23</td>
<td>-3.24</td>
</tr>
<tr>
<td>QMEAN4 score</td>
<td>0.565</td>
<td>-3.40</td>
</tr>
</tbody>
</table>

If you publish results from QMEAN, please cite the following paper:
<table>
<thead>
<tr>
<th>TARGET</th>
<th>1</th>
<th>VKEALFMN GGEVESSYAQ HARSTKIVTS ITKPILNAV HSLFSEDPH-</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>3</td>
<td>lqevlhmm gt----syak nssynlflfli- rvkpvlqegci gellranlpi</td>
</tr>
<tr>
<td>TARGET</td>
<td>44</td>
<td>hhh h hhhhhhhh hhhhh</td>
</tr>
<tr>
<td>2efjA</td>
<td>44</td>
<td>hhh h h hhhhhhhhhh hhhhh</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>48</th>
<th>RKKVLNVDAL GCAAGPNFPS VILTVKESLE RKCKELNCQP PELQVYLNDSL</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>50</td>
<td>inkcfkvgd gcaasqpntfs tvrdivqsid -------kv ptigiflnld</td>
</tr>
<tr>
<td>TARGET</td>
<td>58</td>
<td>sssssss s hhh hhhhhhhhh hhhhh sssssss</td>
</tr>
<tr>
<td>2efjA</td>
<td>58</td>
<td>sssssss s hhh hhhhhhhhhh sssssss</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>98</th>
<th>PGNDFNSLFK DLSRVGED-- -QKSDVLLPC FVMGAPGSFY GRLFPRSLMLH</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>102</td>
<td>fqndfnsvfk llpsfyrnle kengrkigsc ligampsfsy srlfpeesmh</td>
</tr>
<tr>
<td>TARGET</td>
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<td>hhhhh hhhhhhhhh hhh hhhhhhhhh</td>
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<tr>
<td>2efjA</td>
<td>116</td>
<td>hhhhh hhhhhhh hh sssssss</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>145</th>
<th>LVHSSYSVHW LSQPVKGLTS KEBGPLNKGK IYISKTSPPV VAAAYLAQFK</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>152</td>
<td>flhsyclhw lsqvpsgi-- ----svnkgc iysskasrpp igkayldqft</td>
</tr>
<tr>
<td>TARGET</td>
<td>166</td>
<td>ss sssssss sss sssssss</td>
</tr>
<tr>
<td>2efjA</td>
<td>166</td>
<td>ss sssssss h hhhhhhhhhh</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>195</th>
<th>EDFTLLLKSR AEEMVQNGRM VLILHGRQAS DPMGKESCYH WEILABAEISE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>202</td>
<td>kdfttflrih seelisgrnm lltfickede fd----hpns mdlemsind</td>
</tr>
<tr>
<td>TARGET</td>
<td>216</td>
<td>sssssss sss sssssss h hhhhhhhhh</td>
</tr>
<tr>
<td>2efjA</td>
<td>216</td>
<td>sssssss sss sssssss h hhhhhhhhh</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>245</th>
<th>MVSGLLVDEE KLDSFNVPYY TPLQEEVQDI VDKEGSFAVE HIETFTLDLV</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>248</td>
<td>lvieghleee kldsfnpvpi apsteevkri veegsfei lyltfnapyd</td>
</tr>
<tr>
<td>TARGET</td>
<td>262</td>
<td>hhh h h hhh sss sssssss h hhhhhhhhh</td>
</tr>
<tr>
<td>2efjA</td>
<td>262</td>
<td>hhh h h hhh sss sssssss h hhhhhhhhh</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>295</th>
<th>DKQESD--- -TRAKGEQLA KNIRCUTESI ISYQFGKTEIT EKVYHKLTQI</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>298</td>
<td>agfsispvsc deharaahva svvsiyepi lashtgeail pdlshriakn</td>
</tr>
<tr>
<td>TARGET</td>
<td>312</td>
<td>hhhhhhh hhhhh hh h hhhh h h h hh hh hhhhhhhhh</td>
</tr>
<tr>
<td>2efjA</td>
<td>312</td>
<td>hh h hhhhhhhhh hh hh hh hh hh hh hh hh hh</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TARGET</th>
<th>340</th>
<th>VVKDMASRPP TNTTVVVLSS RT</th>
</tr>
</thead>
<tbody>
<tr>
<td>2efjA</td>
<td>357</td>
<td>aakvrlsgkg fydsviisla kkp</td>
</tr>
<tr>
<td>TARGET</td>
<td>374</td>
<td>sssssssss s</td>
</tr>
<tr>
<td>2efjA</td>
<td>374</td>
<td>sssssssss s</td>
</tr>
</tbody>
</table>

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Alignment:
Modeling Log:

3.70 (SP3)
Loading Template: 2efjA.pdb
Loading Raw Sequence
Loading Alignment: ./NXXX.align.submit.fasta
Removing HET groups from template structure
Refining Raw Sequence Alignment
ProModII: doing simple assignment of backbone
ProModII: adding blocking groups
Adding Missing Sidechains
AddPolar H
BuildDeletedLoopsModel

community problem (C-N > 3.0A) at residue: 11
Trying Ligating with anchor residues ASN 8 and GLU 11
Trying Ligating with anchor residues ASN 8 and VAL 12
Trying Ligating with anchor residues ASN 8 and GLU 13
Trying Ligating with anchor residues ASN 8 and SER 14
Trying Ligating with anchor residues ASN 8 and SER 15
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues MET 7 and SER 15
Number of Ligations found: 500
ACCEPTING loop  210: clash=   0 FF=        297.4 PP=  2.00
Trying Ligating with anchor residues PHE 46 and LYS 49
Number of Ligations found: 7
ACCEPTING loop  2: clash=   0 FF=       -278.4 PP= -2.00
community problem (C-N > 3.0A) at residue: 89
Trying Ligating with anchor residues GLN 86 and GLU 89
Trying Ligating with anchor residues CY5 85 and GLU 89
Trying Ligating with anchor residues ASN 84 and GLU 89
Trying Ligating with anchor residues LEU 83 and GLU 89
Trying Ligating with anchor residues GLY 82 and GLU 89
Trying Ligating with anchor residues LYS 81 and GLU 89
Trying Ligating with anchor residues CY5 80 and GLU 89
Trying Ligating with anchor residues LYS 79 and GLU 89
+++ Warning: Ligation Failed, SparePart will be inserted later
+++ It is usually the sign that the region is misaligned.
Trying Ligating with anchor residues ASP 115 and SER 118
Number of Ligations found: 5
ACCEPTING loop  3: clash=   0 FF=       1162.3 PP= -3.00
community problem (C-N > 3.0A) at residue: 163
Trying Ligating with anchor residues LYS 160 and THR 163
Trying Ligating with anchor residues LYS 160 and SER 164
Trying Ligating with anchor residues LYS 160 and LYS 165
Trying Ligating with anchor residues LYS 160 and GLU 166
Trying Ligating with anchor residues LYS 160 and GLY 167
Trying Ligating with anchor residues LYS 160 and LEU 168
Trying Ligating with anchor residues LYS 160 and PRO 169
Number of Ligations found: 500
ACCEPTING loop  174: clash=   0 FF=       32.0 PP= -4.00
community problem (C-N > 3.0A) at residue: 301
Trying Ligating with anchor residues GLU 298 and THR 301
Trying Ligating with anchor residues GLU 298 and THR 301
Number of Ligations found: 15
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues LYS 296 and THR 301
Number of Ligations found: 147
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ASP 295 and THR 301
Number of Ligations found: 63
ACCEPTING loop  31: clash=   0 FF=       1162.3 PP= -3.00
Small Ligation (C-N <3.0A) ignored;
GROMOS will repair it at residue THR 302
Building CSP loop with anchor residues THR 27 and THR 30
Number of Ligations found: 8
ACCEPTING loop  0: clash=   0 FF=       263.7 PP= -1.00
Building CSP loop with anchor residues PRO 226 and SER 231
Number of Ligations found: 30
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues PRO 226 and CYS 232
Number of Ligations found: 500
ACCEPTING loop 308: clash= 0 FF= 195.7 PP= -1.00
Finding Spare-Part loop with anchor residues GLU 77 and PRO 88
connectivity problem --> including residue PRO 89
Finding Spare-Part loop with anchor residues GLU 77 and GLU 89
ACCEPTING loop 72 from 8ABP_ Clash= 2 FF= -53.0 PP=120.73
BadPhi= 1 BadGX= 0 BadXP= 1 weakXP= 1 Score= 4.75 rms= 0.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 47)
Final Total Energy: -10339.067 KJ/mol
Dumping Sequence Alignment

Template Selection Log:

- Start SMR-Pipeline in automated mode on BC2-cluster at Wed Feb 12 01:14:21 2014
- User specified template structure by a PDB identifier(2efjA), entering user template mode
- Aligning sequence of the user template structure with the target sequence using BLAST
  - Alignment quality between target and specified template is too low
- Aligning sequence of the user template structure with the target sequence using HHSearch
  - Send 1 target-template alignments for modeling
  - *******************************************************************************
  - building model based on 2efjA (3-363) was successfull
- Workspace Pipeline parameter
  Cut-off parameters to model the target based on a BLAST target-template alignment
  Evalue : 0.0001
  Minimum Template size (aa) for ranking : 25
  Minimum Sequence identity : 60

  Cut-off parameters to model the target based on a HHSearch target-template alignment
  Evalue : 0.0001
  Probability : 50
  MAC : 0.3

  Parameters for model selection
  Minimal number of uncovered target residues after BLAST to run HHSEARCH : 50
  Minimal number of uncovered target residues to model an additional template : 25
- Finish SMR-Pipeline in automated mode on BC2-cluster at Wed Feb 12 01:42:07 2014

Quaternary Structure Annotation of the Template
2efj is annotated as DIMER
The oligomeric state of the structure was assigned by the authors of the corresponding PDB entry
The following biological unit was used to build the template structure: 2efj.pdb1.gz

Quaternary Structure Modelling of the Target Protein
The target and template sequences are too diverse (seqid: 34.324) to infer a conservation of the oligomeric state
Please use the advanced features of the SwissModel Project Mode
The target structure was calculated as SINGLE CHAIN

**Ligand Modeling Log: Template’s ligands section**

Ligands in the template: 37T: 1, ALA: 1.

The template contains ligands that are not yet part of the pipeline. Ligands which are currently assessed are listed in the help page.

No ligands were included in the model.

**References:** If you publish results using SWISS-MODEL, please cite the following papers: